

NON-EQUILIBRIUM CHEMISTRY IN THE SOLAR NEBULA AND EARLY SOLAR SYSTEM: IMPLICATIONS FOR THE CHEMISTRY OF COMETS Bruce Fegley, Jr., Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA 02139 USA

Theoretical models of solar nebula and early solar system chemistry which take into account the interplay between chemical, physical, and dynamical processes have great utility for deciphering the origin and evolution of the abundant chemically reactive volatiles (H, O, C, N, S) observed in comets. In particular, such models are essential for attempting to distinguish between presolar and solar nebula products and for quantifying the nature and duration of nebular and early solar system processing to which the volatile constituents of comets have been subjected. This talk will focus on the diverse processes and energy sources responsible for chemical processing in the solar nebula and early solar system. The processes to be considered include homogeneous and heterogeneous thermochemical and photochemical reactions, and disequilibrium resulting from fluid transport, condensation, and cooling whenever they occur on timescales shorter than those for chemical reactions. The energy sources to be considered include the thermal energy of the nebula, shock waves and photons from lightning discharges, proto-solar and stellar photons, and radioactive decay processes. Plausible models for the chemical compositions of gases and volatile-bearing grains as a function of space and time in the nebula and in subnebulae around the giant planets will be discussed.

Some conclusions of this theoretical modelling (e.g., see Fegley, 1988; Fegley and Prinn, 1988; Prinn and Fegley, 1988) include the following:

1. Non-equilibrium chemistry was responsible in large part for establishing the chemical speciation in the solar nebula and in subnebulae around the giant planets.
2. The dominant carbon and nitrogen gases in the solar nebula were CO and N_2 . This is probably similar to the situation in the interstellar medium where observations and theoretical models imply that CO and N_2 also dominate the gas phase carbon and nitrogen inventories. In contrast, the dominant carbon and nitrogen gases in giant planet subnebulae were CH_4 and NH_3 .
3. Fe metal grains in the solar nebula catalyzed the formation of organic compounds from nebular $CO + H_2$ via Fischer-Tropsch-type reactions. On the order of 10% of the total CO inventory was converted into organic compounds, in this fashion.
4. Hydrated silicate formation was kinetically inhibited in the solar nebula, but was kinetically favorable in the subnebulae around giant planets. Any hydrated silicates observed in comets, therefore, are *not* solar nebula products.
5. Formation of FeS by the sulfurization of Fe metal grains was kinetically favorable in the solar nebula. In contrast, FeO incorporation into silicates at low

temperatures (e.g., as predicted by canonical equilibrium condensation models) and *bulk* Fe_3O_4 formation were both kinetically inhibited in the solar nebula.

6. Clathrate formation (e.g., CO and N_2 clathrates) was kinetically inhibited in the solar nebula but CH_4 clathrate formation was kinetically favorable in the subnebulae around giant planets.
7. The CO/CH_4 and N_2/NH_3 ratios in comet P/Halley are intermediate between those ratios in the solar nebula ($CO/CH_4 \gg 1$ and $N_2/NH_3 \gg 1$) and in giant planet subnebulae ($CO/CH_4 \ll 1$ and $N_2/NH_3 \ll 1$). These intermediate ratios are most plausibly produced by a two component mixing model in which CO -, N_2 -rich material from the solar nebula (and/or from the interstellar medium) is mixed with a smaller amount of CH_4 -, NH_3 -rich material from subnebulae around the giant planets.
8. Non-equilibrium processing due to lightning discharges and photochemistry driven by stellar photons were potentially significant chemical reprocessing mechanisms in the outer solar nebula. In contrast, photochemistry driven by solar photons was unimportant in the very hot, thermochemically-controlled inner nebula. Absorption by gas and dust also limited severely the importance of solar UV photochemistry in the outer regions of the solar nebula. Dust absorption played a similar limiting role during early solar system history.
9. Deuterium-to-hydrogen ratios significantly higher than the canonical primordial value of $D/H \sim 2 \times 10^{-5}$ (e.g., the terrestrial $D/H \sim 1.6 \times 10^{-4}$) cannot be produced by low temperature equilibration in the solar nebula.

These conclusions, as well as their implications for the chemistry of comets will be discussed in more detail at the meeting. Recommendations for specific tests of these implications will also be made.

References

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